Materials Science WS #1

Molecular Orbital Theory

1. a.) Draw an energy level diagram for the H2-1 ion.

b.) Write the electron configuration of the ion in terms of its MOs.

c.) Calculate the bond order in H2-1

d.) Suppose that the ion is excited by light, so that an electron moves from a

lower-energy to a higher-energy molecular orbital. Would you expect the excited-state H2-1 ion to be stable or to fall apart?

2. Which of the following ions would you expect to be diamagnetic: N2-2, O2-2. Be2+2,

C2-1

3. If we assume that the energy-level diagrams for homonuclear diatomic molecules

shown in Figure 9.43 can be applied to heteronuclear diatomic molecules and ions,

predict the bond order and magnetic behavior of:

a.) CO+1

b.) NO-1

c.) OF+1

d.) NeF+1

4. Carbon monoxide, CO, is isoelectronic to N2.

a.) Draw a Lewis structure for CO that satisfies the octet rule.

b.) Assume that the diagram in Figure 9.49 can be used to describe the MOs of

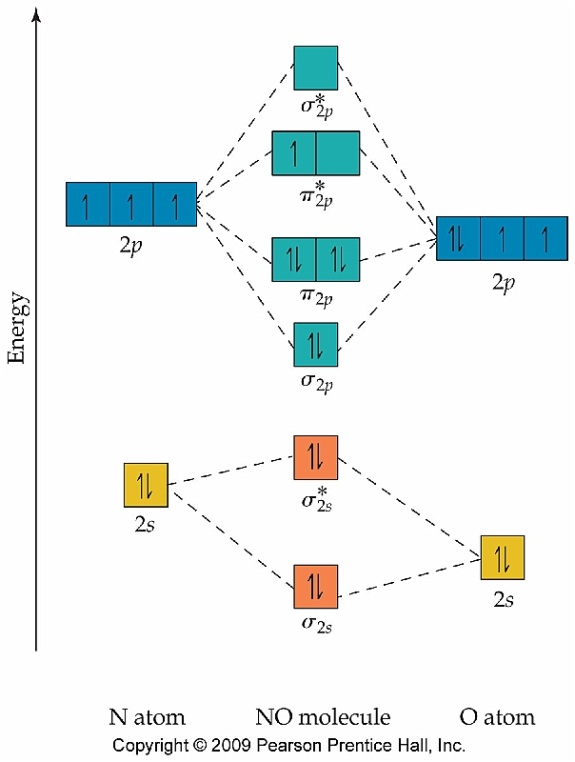
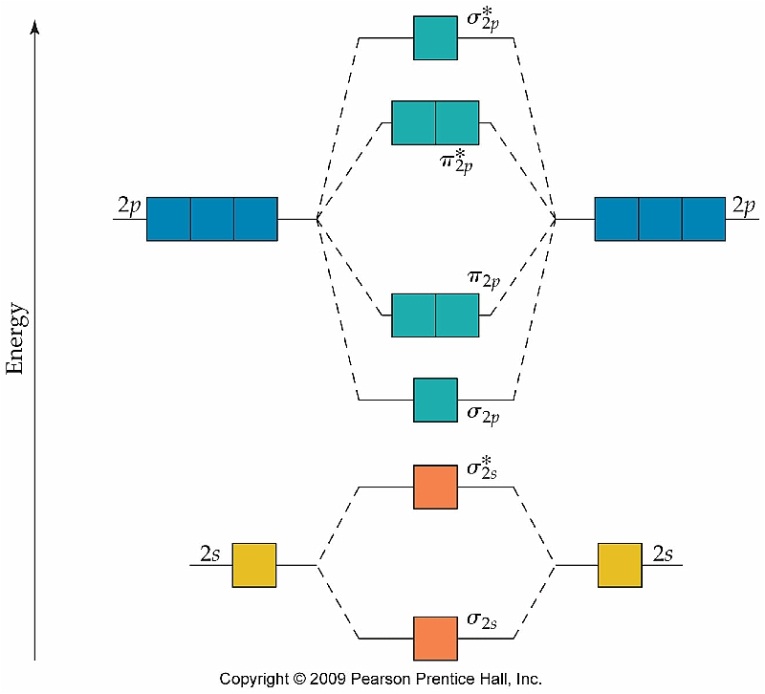
CO. What is the predicted bond order for CO? Is this answer in accord with

the Lewis structure you drew in part a.)?

c.) Experimentally, it is found that the highest-energy electrons in CO reside in a

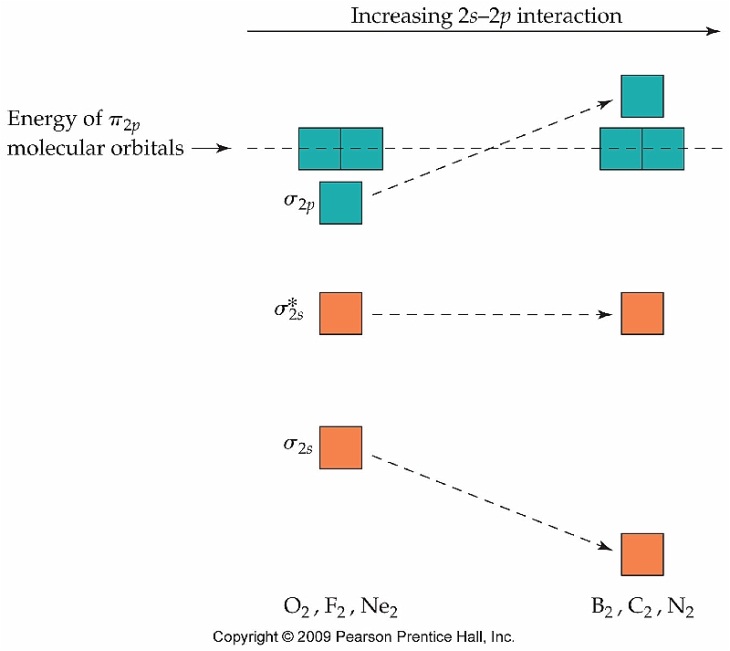
σ-type MO. Is that observation consistent with Figure 9.49? If not, what

modification needs to be made to the diagram? How does this figure relate to   
 Figure 9.45?



**Figure 9.49**

**Figure 9.43**



**Figure 9.45**

**Figure 9.45**